

1,3-diphenyl-1,3-diazetidine
74949-76-1 | DTXSID60321268

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.89 | 0.25 | 0.88 | 0.26 | 0.75 | 0.38 |

Model Results

Predicted value: 10.9 days

Global applicability domain: Outside

Local applicability domain index: 3.58e-01

Confidence level: 7.23e-01

Nearest Neighbors from the Training Set

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1,2-Dimethylcyclohexane

Measured: 777

Predicted: 10.2

[Image not found](#)

Hexane, 2,2,5-trimethyl-

Measured: 777

Predicted: 17.4

[Image not found](#)

1,2,3-Trimethylbenzene

Measured: 24.3

Predicted: 4.97

[Image not found](#)

Cumene

Measured: 511

Predicted: 11.8